Efficient 3D Unstructured Grid Algorithms for Modelling of Chemical Vapour Deposition in Horizontal Reactors

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Abstract

The paper deals with the use of 3D unstructured grid algorithms with adaptive local grid refinement for the computation of flow, heat and mass transfer and their application to the modelling of metalorganic chemical vapor deposition (MOCVD) of epitaxial layers of GaAs and GaN. It is shown that this approach is promising for an accurate 3D modelling of the deposition processes.

1. Introduction

At the growth conditions practically used for MOCVD of GaAs and GaN in horizontal tube reactors, high temperature and species concentration gradients are formed near the hot susceptor and the substrate on it. This is especially critical for the growth of GaN in N_2-ambient. Accurate calculation of the temperature and species concentration gradients is necessary to reproduce experimental observations and to perform optimization of the processes. Commercially available general software packages usually are not efficient enough with respect to execution time and memory requirements.

Unstructured grids were extensively used during the last decade to solve fluid flow problems, the main attention is paid to the development of 2D and 3D solvers for Euler (for example, [1]) and compressible Navier–Stokes [2] equations. The latter approach has also been implemented for the simulation of flow and deposition in CVD reactors [3]. It is also possible to use hybrid unstructured/structured grids combining the flexibility of the former with the high accuracy of the latter in computing the wall friction and heat transfer due to the possibility to align the grid lines to the solid surfaces [4]. The easiness of adaptive grid refinement is a promising feature of this approach for modelling of processes with significantly localized areas of high gradients of parameters.

2. Mathematical model

Flows in epitaxial reactors are characterized by 1) low velocities (compared to the sound speed) and 2) large temperature (and, hence, density) variations. Numerical integration of the compressible Navier–Stokes equations for very low Mach numbers presents severe problems in practice while the well-known Boussinesq approximation is invalid when the density (temperature) variations are comparable or greater than the mean values. In the present work the so-called low-Mach number Navier-Stokes equations are used [5]. The equations in dimensionless form for flows in an open system can be written as

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \vec{V}) = 0 \tag{1}$$

$$\frac{\partial \varrho \vec{V}}{\partial t} + \nabla \cdot (\varrho \vec{V} \vec{V}) = -\nabla P + \frac{1}{Fr} \varrho \vec{j} + \frac{1}{Re} \left[2Div(\mu \dot{S}) - \frac{2}{3} \nabla (\mu \nabla \cdot \vec{V}) \right] \tag{2}$$

$$\varrho \frac{dT}{dt} = \frac{1}{RePr} \nabla \cdot (\lambda \nabla T) \tag{3}$$

$$\varrho T = 1 \tag{4}$$

where ϱ is the density, $\vec{V}$ is the velocity, P is the excess pressure, T is the temperature, μ is the dynamic viscosity, λ is the thermal conductivity, $\dot{S}$ is the deformation rate tensor, $\vec{j}$ is the unit gravitational vector, γ is the ratio of specific heats, $Re = \frac{\varrho_0 V_0 L_0}{\mu_0}$, $Pr = \frac{\mu_0 C_p}{\lambda_0}$, $Fr = \frac{V_0^2}{g L_0}$ are Reynolds, Prandtl and Froude numbers, respectively, C_p is the specific heat at constant pressure. The subindex "o" refers to the values chosen as the scales.

The growth process at practically used growth conditions is limited by the mass transport of Ga-species to the substrate, therefore, a simplified model of the deposition process similar to [5,6] is used in the present work.

$$\frac{\partial \varrho C_i}{\partial t} + \nabla \cdot (\varrho \vec{V} C_i) = \frac{1}{ReSc_i} \nabla \cdot [\varrho (\nabla C_i + C_i K_{T_i} \nabla \ln T)] + W_i \tag{5}$$

3. Numerical method

The Watson incremental triangulation technique, generalized for the 3D case, is the basis for the grid generation method needed to produce a starting grid. The geometry is defined by a surface triangulation and the density of the grid nodes at the surface controls the grid non-uniformity in the volume of the reactor. Grid smoothing and edge swapping algorithms are employed to improve the initial grid quality.

The approximation of the basic equations is performed exploiting Ostrogradskii–Gauss and related integral theorems applied to control volumes around each vertex and to tetrahedral cells themselves to compute viscous terms. The difference equations are solved by simultaneous pointwise relaxation.

In general, refinement methods can be developed in order to minimize either the execution time or the memory requirements. Usually the memory needed for storing the grid information is larger (and sometimes substantially) than that for storing the flow variables. It may be over 50 words per tetrahedron (or over 250 per vertex) [7]. In the present approach an attempt is made to minimize the memory requirements (paying by a higher execution time for reconstruction of grid connectivity and neighbor

relations). Additional improvement results from the fact that only grid refinement and no de-refinement is allowed. The refinement of the current tetrahedron results in introducing nodes in the neighbour tetrahedra having common face (they will be referred to as t–neighbours below) and common edge (e–neighbours). The algorithm is based on strict conventions for the grid elements numbering that allows for a reduction of the memory requirements to about 20 integer words per tetrahedron and to minimize the execution time for the reconstruction of the grid structure. It can be summarized as follows:

1. Mark all tetrahedra for refinement.
2. If the fraction of tetrahedra to be refined does not belong to the given range, change the refinement criterium and repeat step 1^o.
3. For each marked tetrahedron loop through all edges:
   (a) introduce new vertex.
   (b) introduce new vertex into e–neighbour tetrahedra.
4. Check all tetrahedra for a number of new nodes
   (a) 6 nodes (marked tetrahedra themself)
   (b) 3 nodes belonging to one face (t–neighbours)
   (c) 1 node (e–neighbours)
   (d) other

   introduce additional nodes to (d) in order to convert them to (a) or (b) cases.
5. If new nodes have been introduced, repeat step 4^o.
6. Set new connectivity relations

   (tetrahedron $\rightarrow$ 4 vertices vertex $\rightarrow$ 1 tetrahedron).
7. Flag deleted tetrahedra and set new neghbour relations

   (tetrahedron $\rightarrow$ 4 tetrahedra).

The solution procedure is repeated after every global refinement of the grid in the whole reactor. The computations are finished when a grid-independent solution is obtained, i.e. when introduction of additional grid volumes changes the solution only within a prescribed accuracy.

4. Results

The flow regimes corresponding to GaAs and GaN MOCVD have been simulated. An example of a computational result for the modelling of MOCVD of GaAs is presented in the Figure 1. Initial (3151 vertices, 11003 tetrahedra) and final (37355 vertices, 190480 tetrahedra) grids are plotted together with the normalized growth rate distribution of the GaAs layer over the susceptor (only one half of the susceptor is shown). The clustering of the grid cells occurs in the regions of high temperature and species concentration gradients where high accuracy of the calculations is required to predict the growth rate distribution. In the parts of the flow where smooth variations of the flow parameters occur a much coarser grid is sufficient to get an accurate solution.

As a conclusion it can be stated that the proposed approach due to its high flexibility is promising for simulations of flow and deposition in CVD reactors.

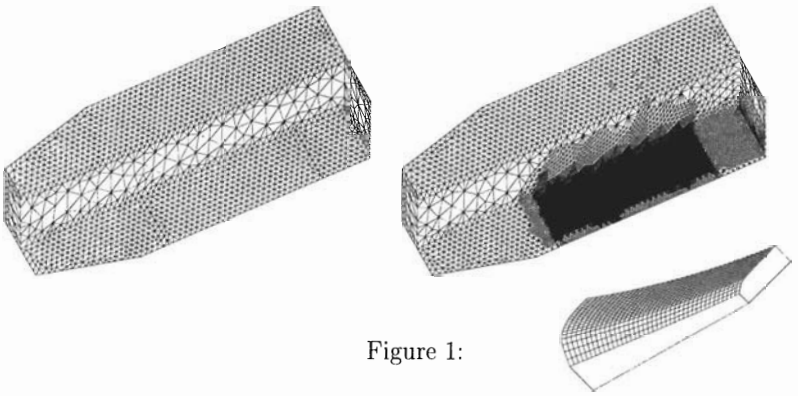

Figure 1:

5. Acknowledgement

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6. References

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